

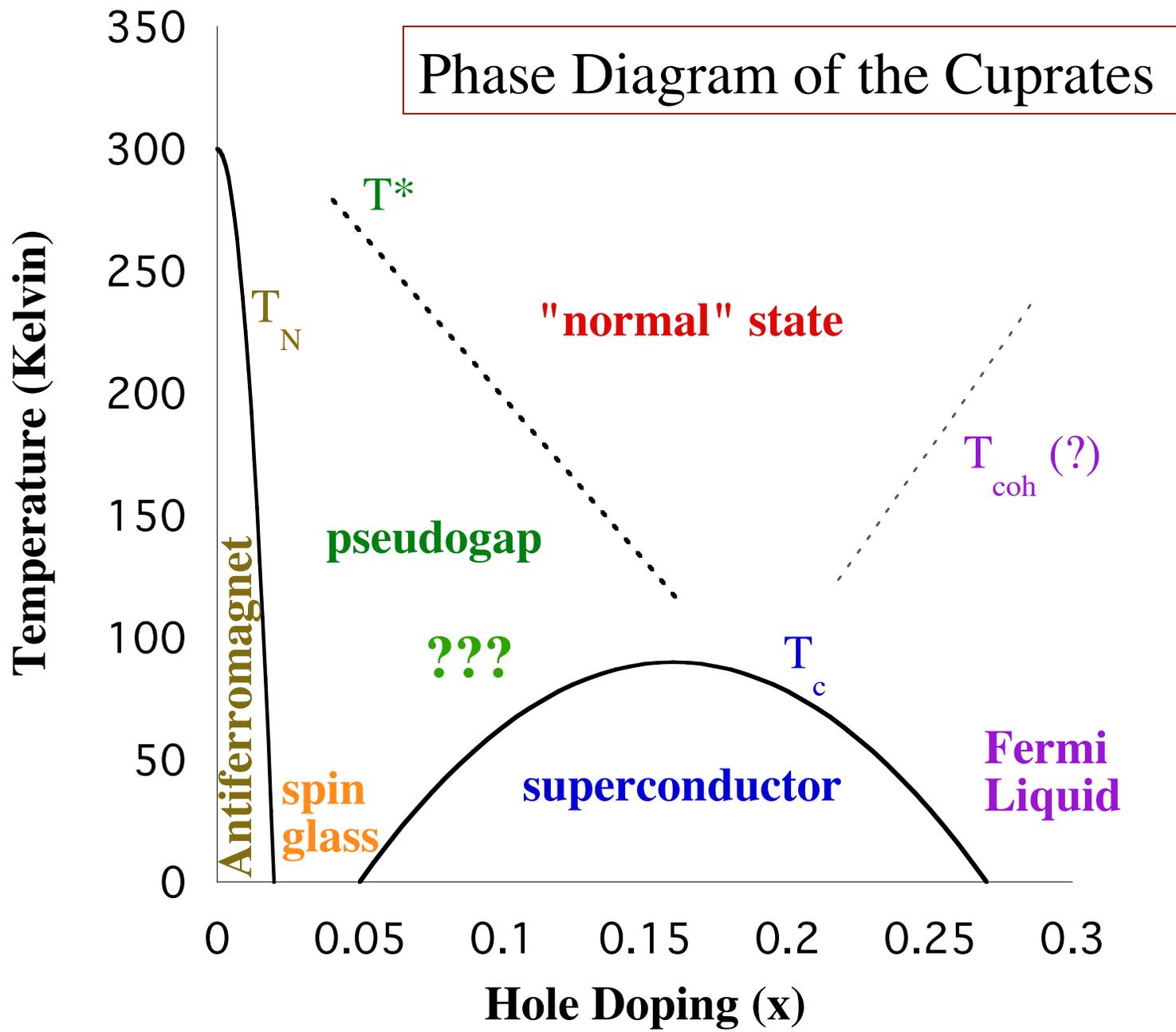
X-Ray Dichroism, Chirality, and Orbital Currents

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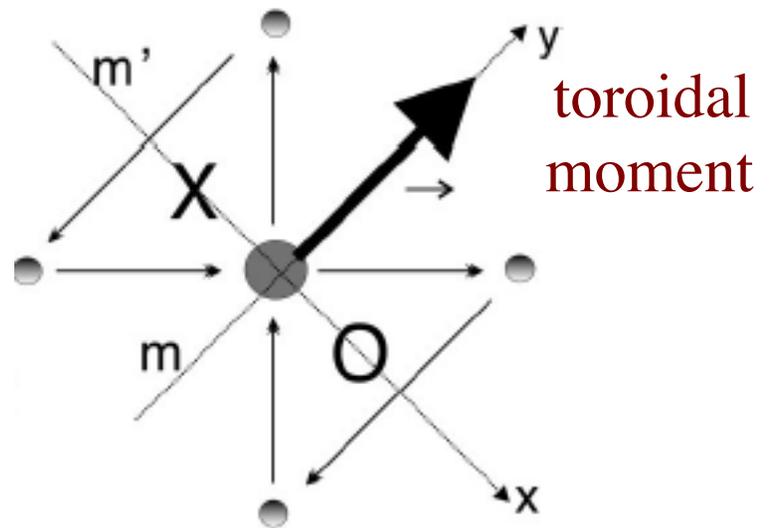
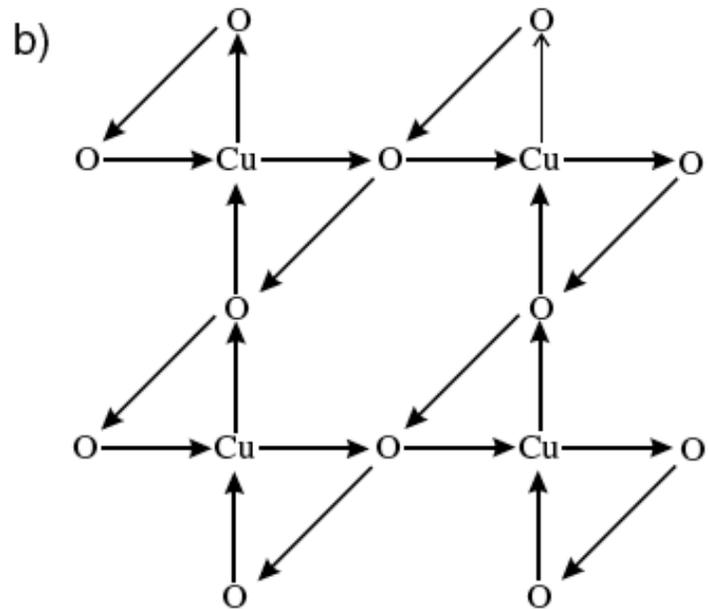
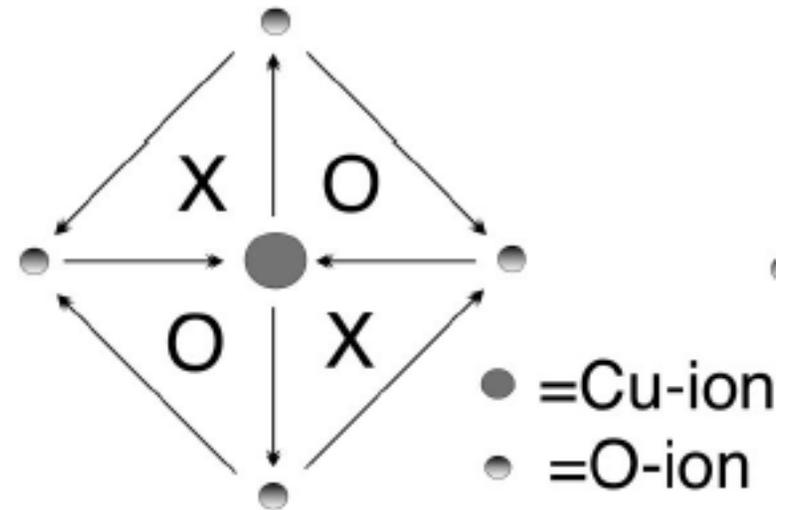
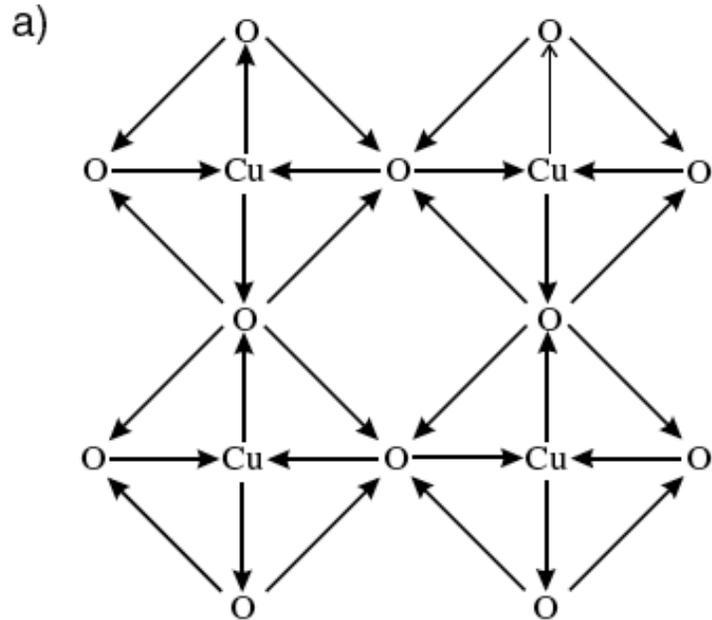
Telluride, July 19, 2013



What is the Pseudogap?

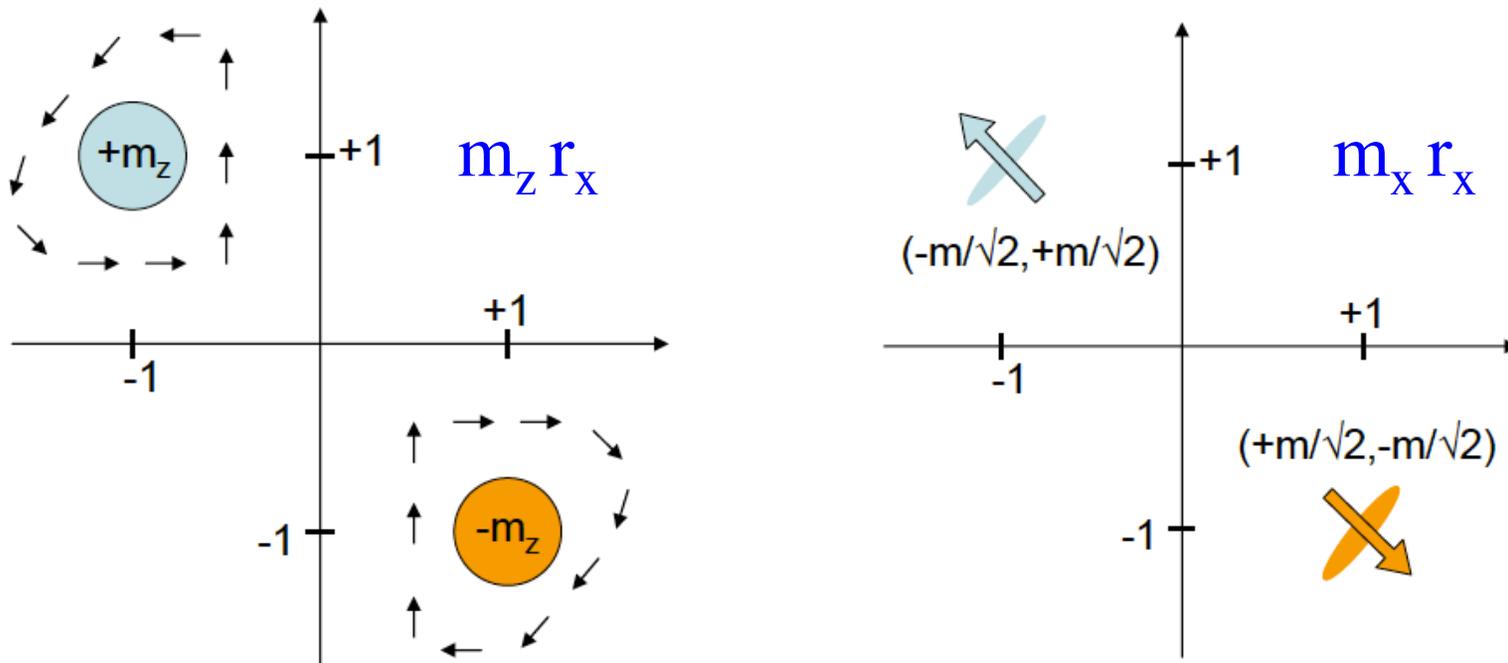
1. Spin singlets
2. Pre-formed pairs
3. Spin density wave
4. Charge density wave
5. d density wave
6. Orbital currents
7. Flux phase
8. Stripes/nematic
9. Valence bond solid/glass
10. Combination?

Orbital Currents



Simon & Varma, PRL (2002)
Di Matteo & Varma, PRB (2003)

Orbital Currents - Combinations of magnetic monopoles, toroidal dipoles & magnetic quadrupoles

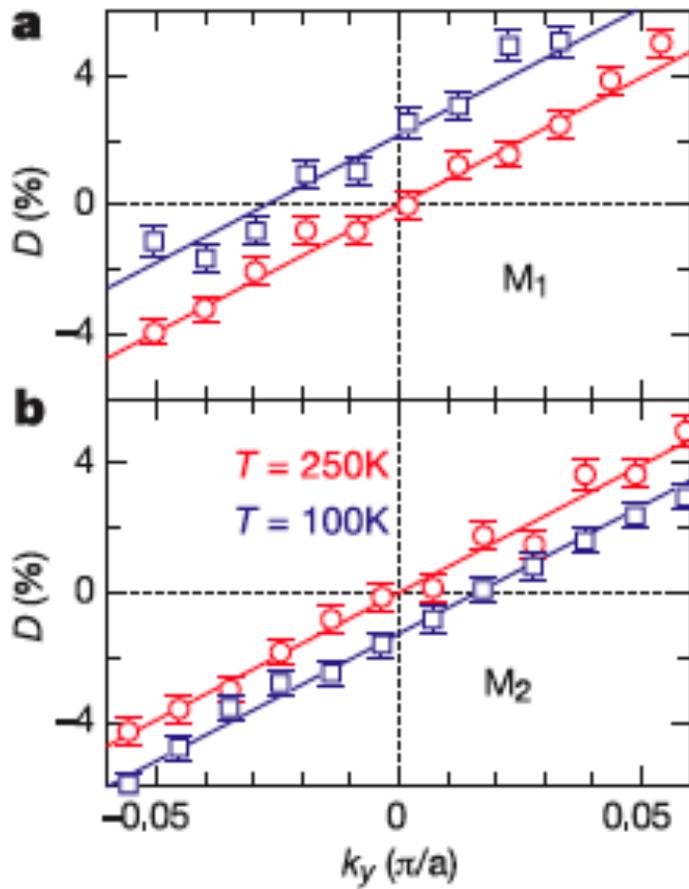


$$M_{ij} \equiv \sum_{\alpha=1,2} \left[m_i^\alpha r_j^\alpha + r_i^\alpha m_j^\alpha - \frac{2}{3} \delta_{ij} \sum_l m_l^\alpha r_l^\alpha \right]$$

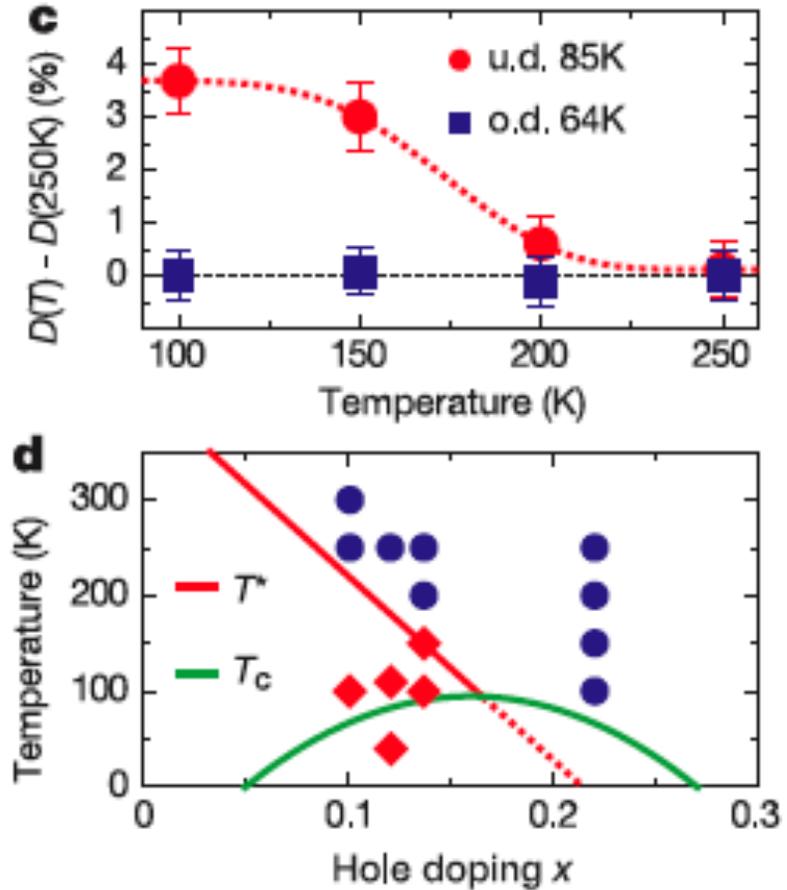
$$T_{ij} \equiv \sum_{\alpha=1,2} [m_i^\alpha r_j^\alpha - r_i^\alpha m_j^\alpha]$$

ARPES dichroism tracks the pseudogap

Question – chirality or time reversal breaking?

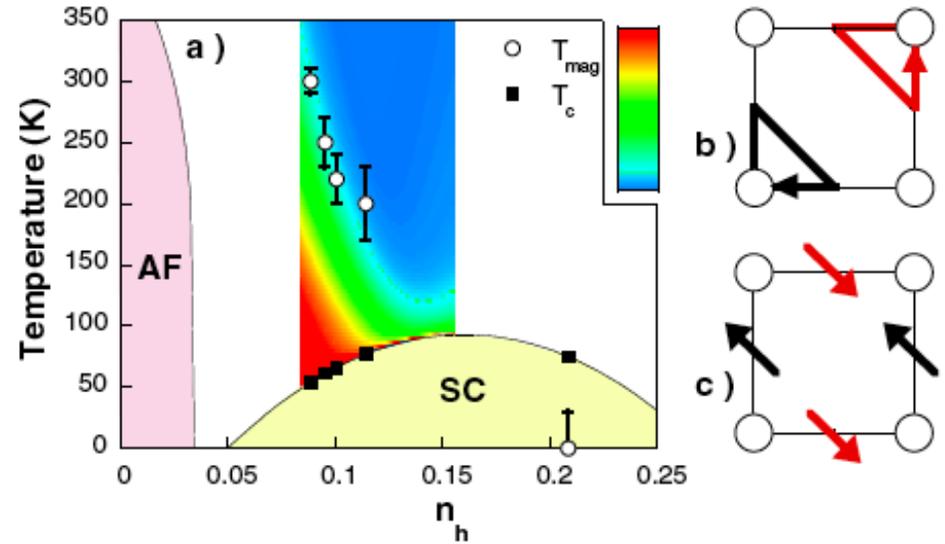
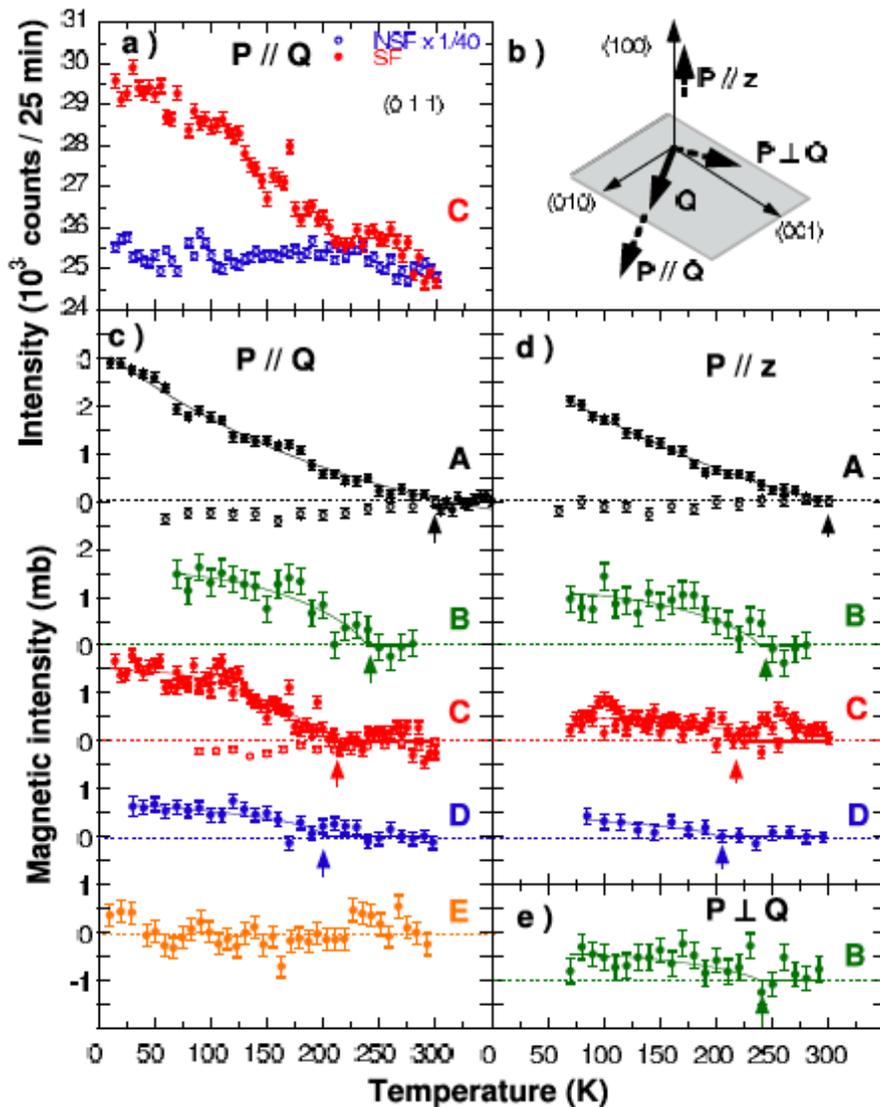


↑
mirror plane



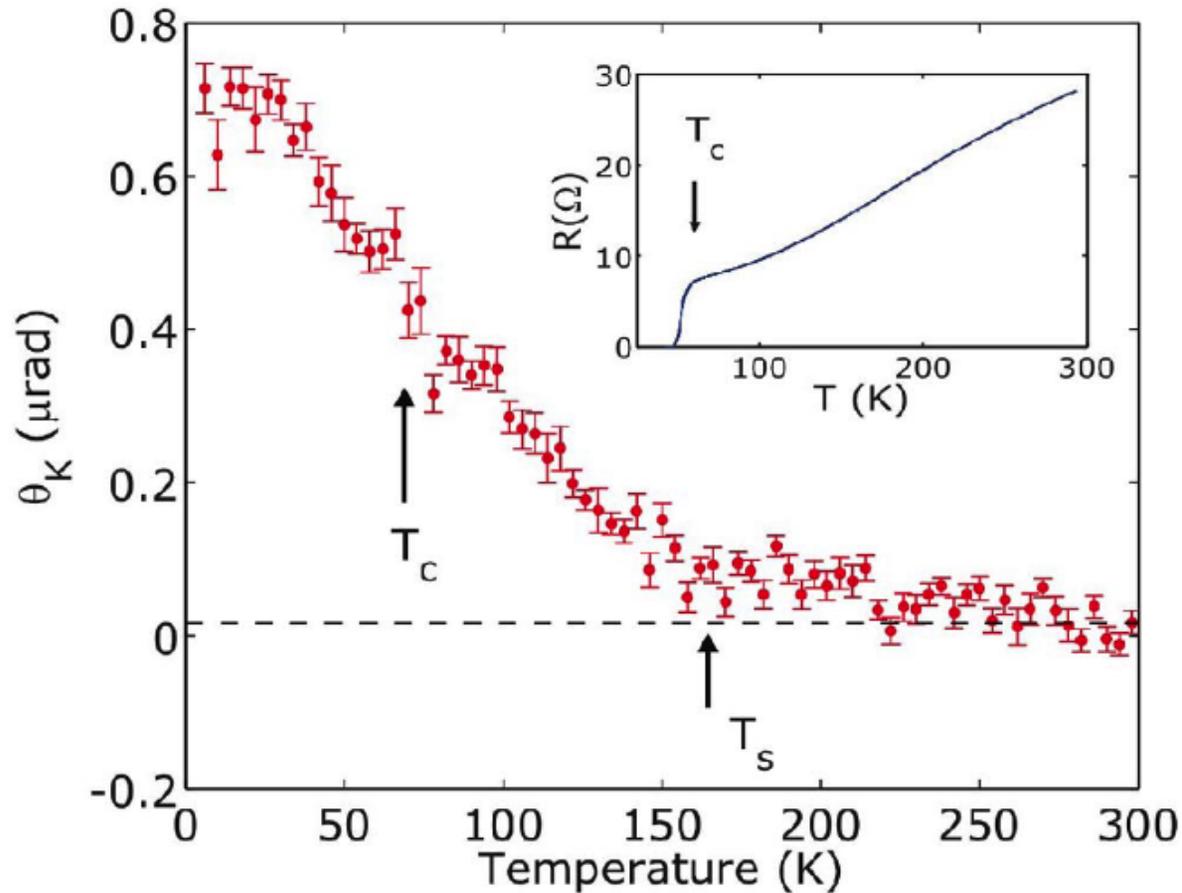
Kaminski *et al.*, Nature 2002

Polarized neutrons see intra-unit cell magnetism



Fauque *et al.*, PRL 2006

Polar Kerr Effect seen as well (time reversal breaking?)



Chirality instead?

Hosur et al, PRB (2013)

Orenstein & Moore, PRB (2013)

Xia et al., PRL 2008

X-ray Optical Activity (E1-E2)

1. X-ray natural circular dichroism (XNCD)

Alagna et al., PRL 1998; *Goulon et al.*, JCP 1998 (LiIO₃)

(time reversal even part of $\sigma^L - \sigma^R$)

2. Non-reciprocal x-ray linear dichroism (NRXLD)

Goulon et al., PRL 2000 (V₂O₃)

(time reversal odd part of $\sigma^{90} - \sigma^0$)

3. X-ray magneto-chiral dichroism (XM χ D)

Goulon et al., PRL 2002 (Cr₂O₃)

($\sigma(\mathbf{H}) - \sigma(-\mathbf{H})$)

4. X-ray non-reciprocal directional dichroism (XNDD)

Kubota et al., PRL 2004 (GaFeO₃)

($\sigma^{90}(\mathbf{H}) - \sigma^{90}(-\mathbf{H})$)

5. X-ray circular intensity differential (XCID)

Goulon et al., JPCM 2007 (ZnO)

(polar vector part of $\sigma^L - \sigma^R$)

Dipole moments in matter

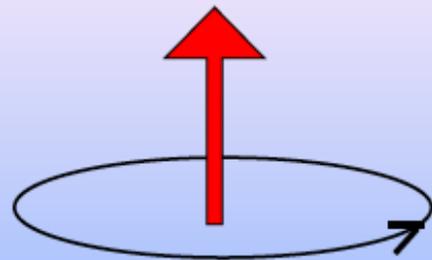
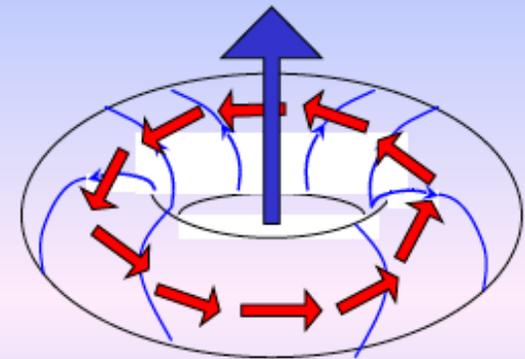
Electric dipole (d)



Polar Toroidal dipole (t)
or anapole

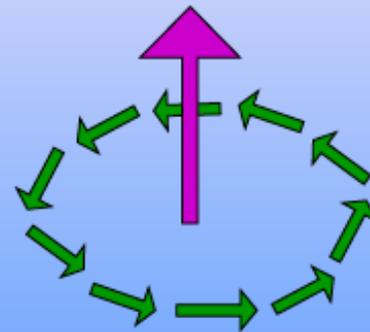
$$\text{as } \mathbf{j} = \text{curl } \mathbf{m}$$

$$\mathbf{t} \equiv -\frac{1}{2} \int \mathbf{r} \times \mathbf{m} \, d\mathbf{r}$$



Magnetic dipole (m)

Axial Toroidal dipole (g)



$$\mathbf{g} \equiv -\frac{1}{2} \int \mathbf{r} \times \mathbf{d} \, d\mathbf{r}$$

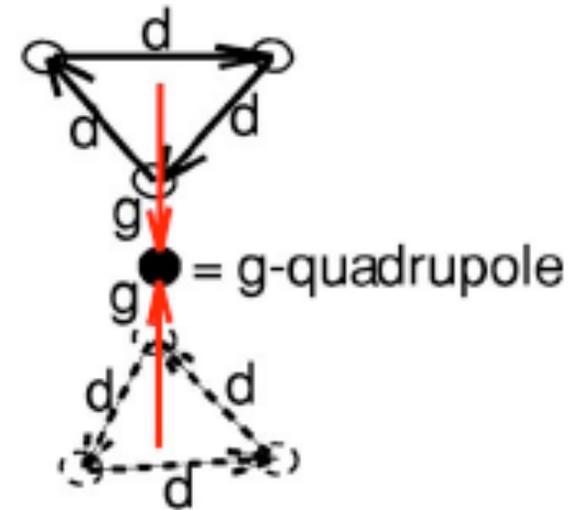
X-ray Natural Circular Dichroism (XNCD)

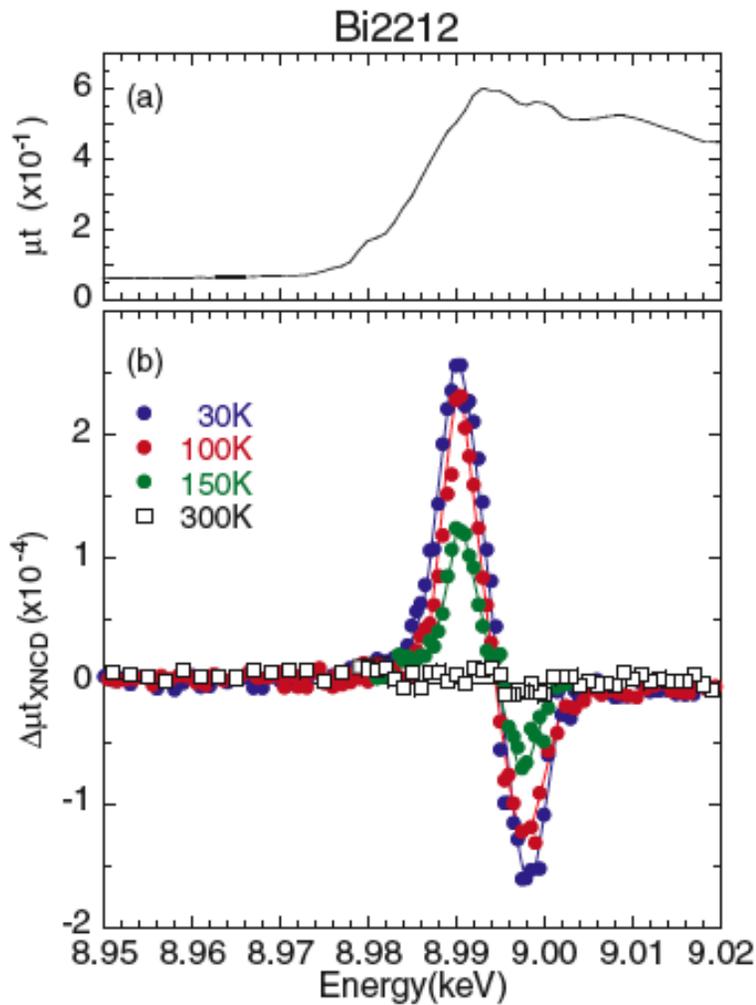
E1-E2 interference (broken inversion symmetry)

$$\vec{L} \cdot (\hat{\epsilon}^* \times \hat{\epsilon}) (\vec{\Omega} \cdot \hat{k})$$

where

- \mathbf{L} is the orbital angular momentum
- \mathbf{k} is the wavevector of the x-ray
- $\boldsymbol{\epsilon}$ is the polarization of the x-ray
- $\boldsymbol{\Omega}$ is the toroidal moment operator



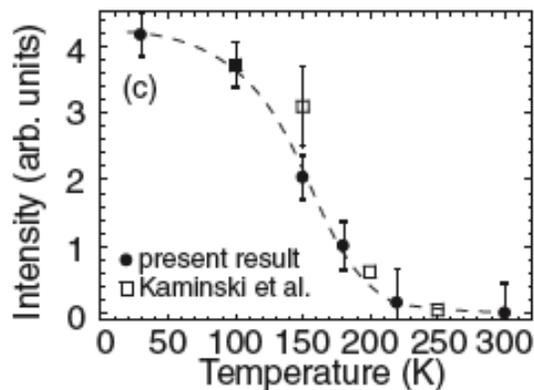


XNCD
 Underdoped Bi2212
 ($T_c = 80\text{K}$)
 Cu K edge

Signal tracks ARPES dichroism

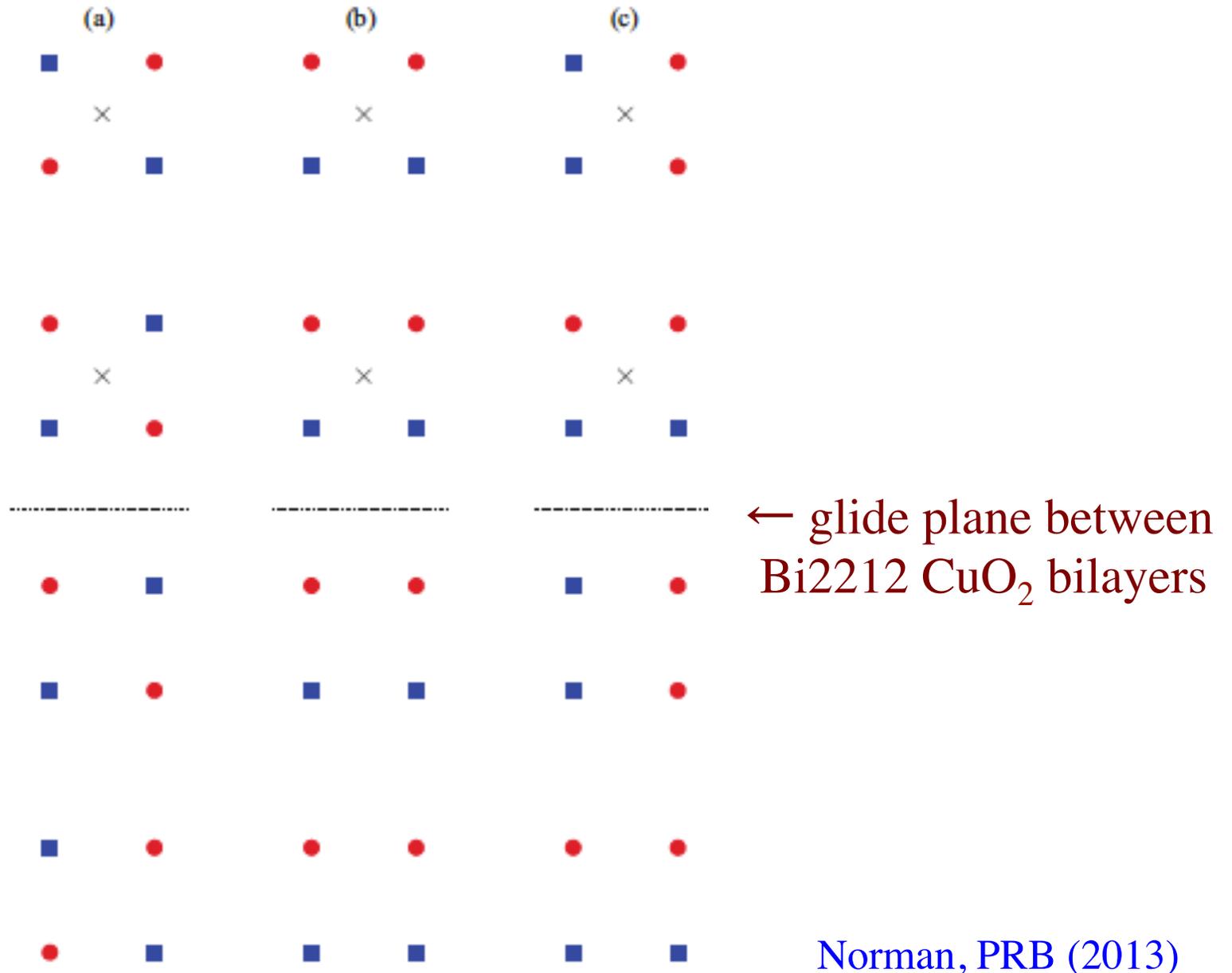
Unusual aspects

1. Simple +/- peak profile
2. Peaks at edge, not pre-edge

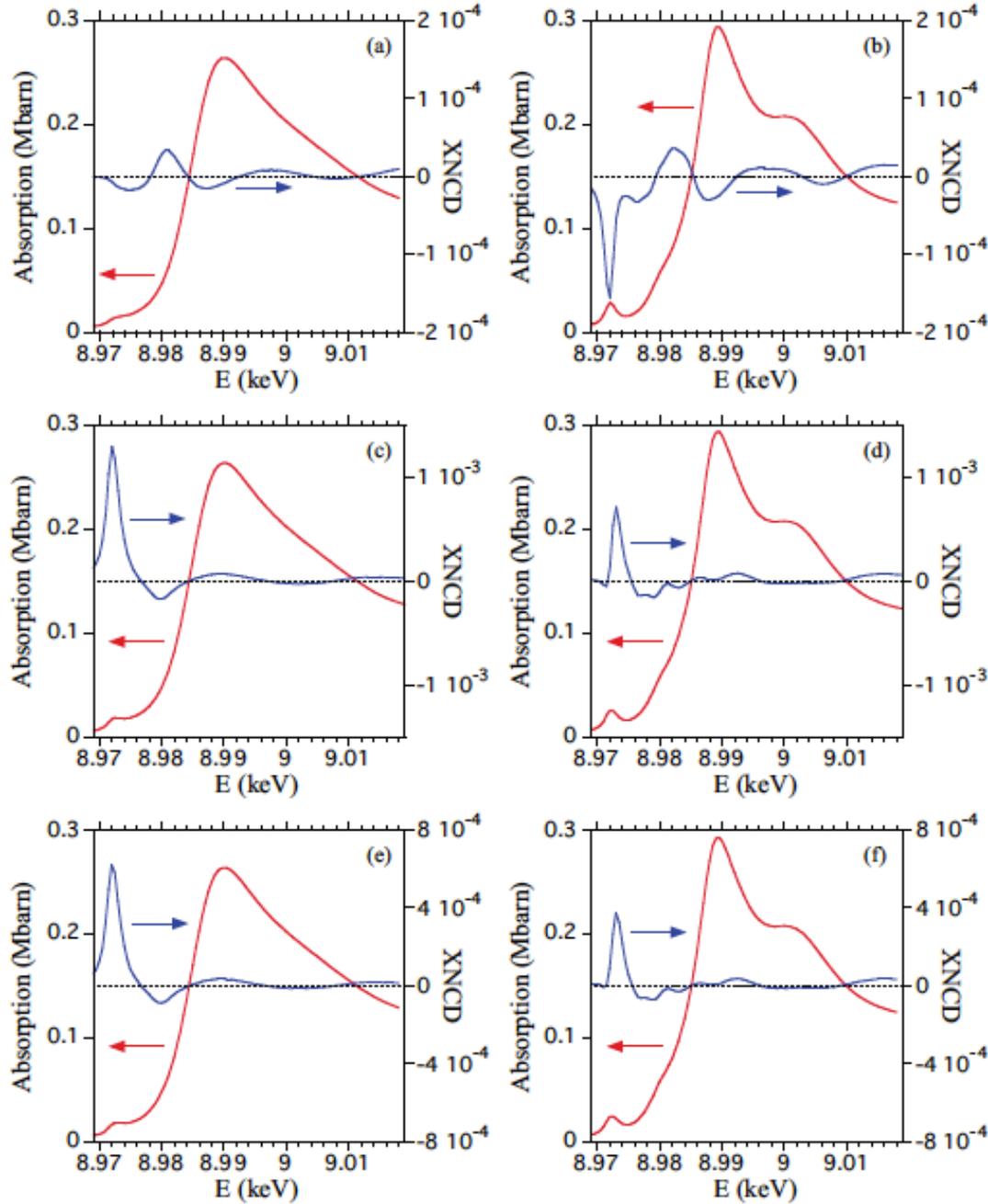


Kubota *et al.*, JPSJ (2006)

Charge Ordering on oxygen sites (blue + vs red -)?

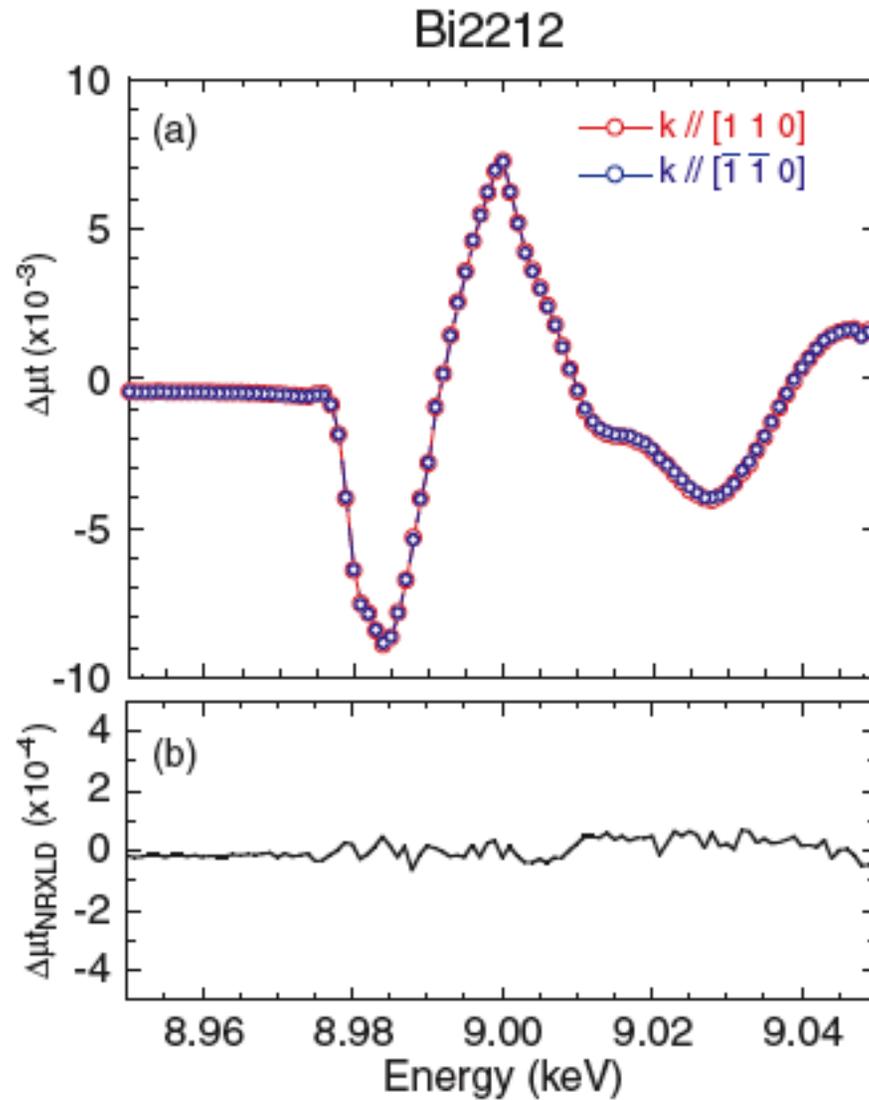


Resulting XNCD signature (Bi2212)

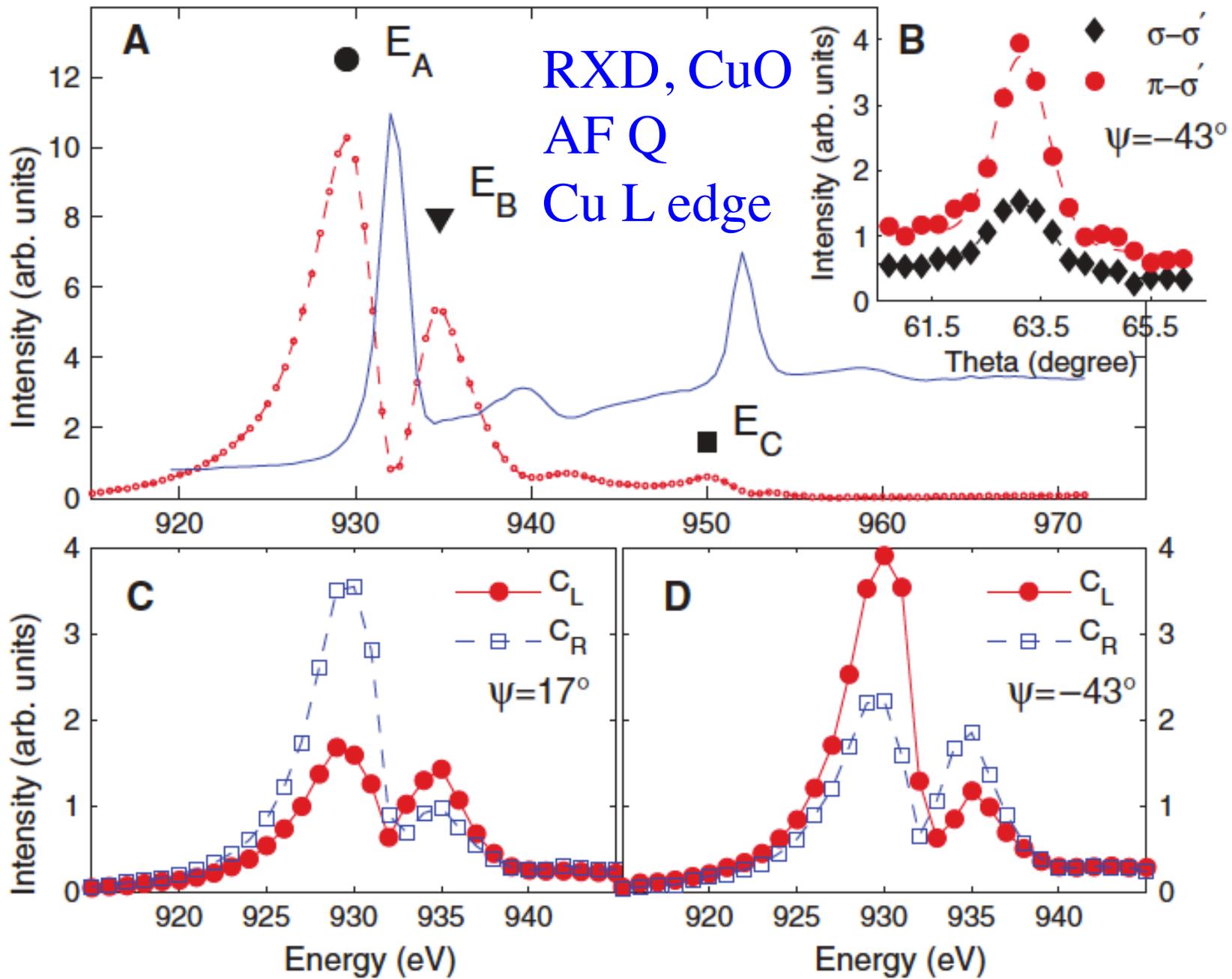


Norman, PRB (2013)

Non reciprocal X ray linear dichroism (null result)

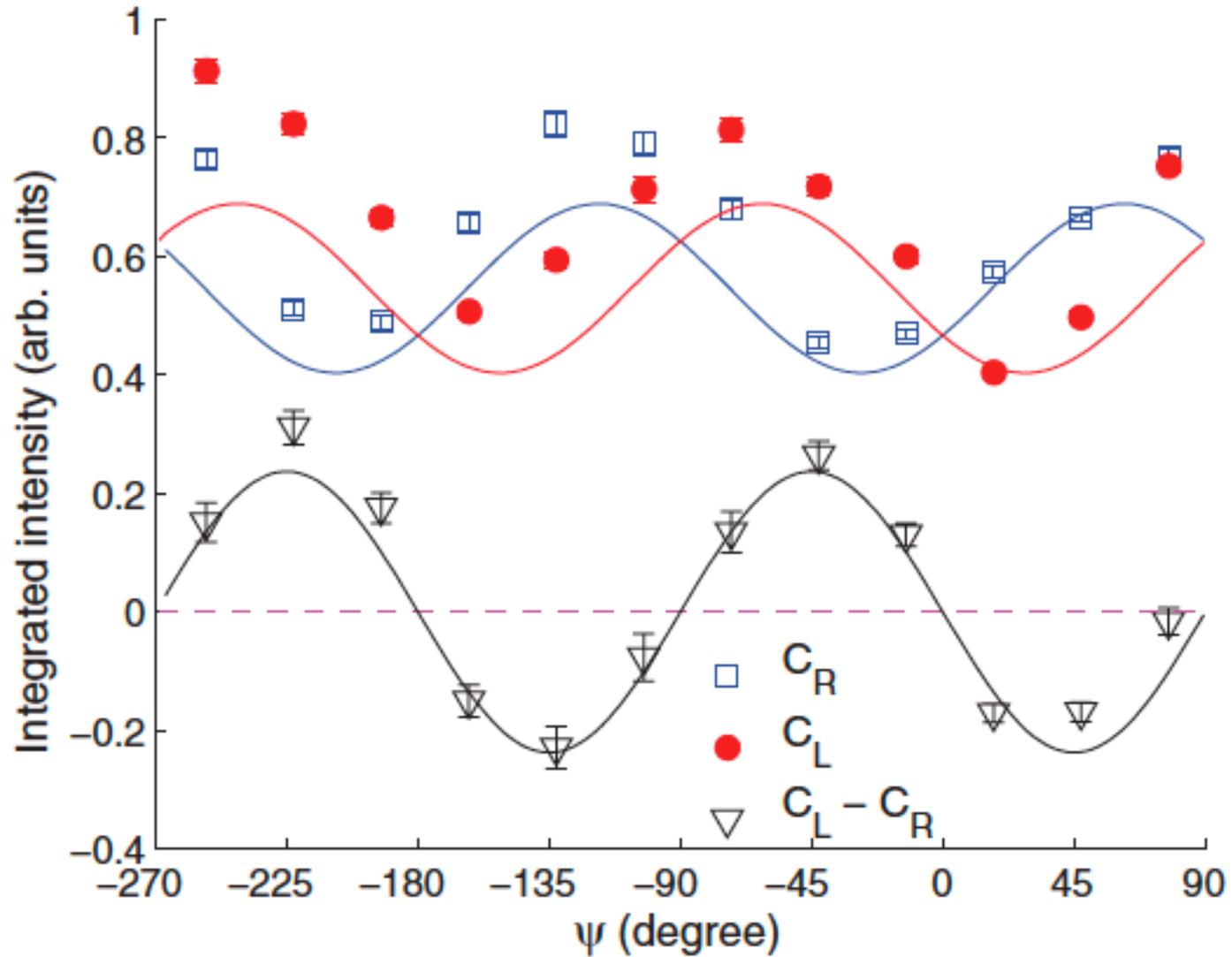


Kubota *et al.*, JPSJ (2006)



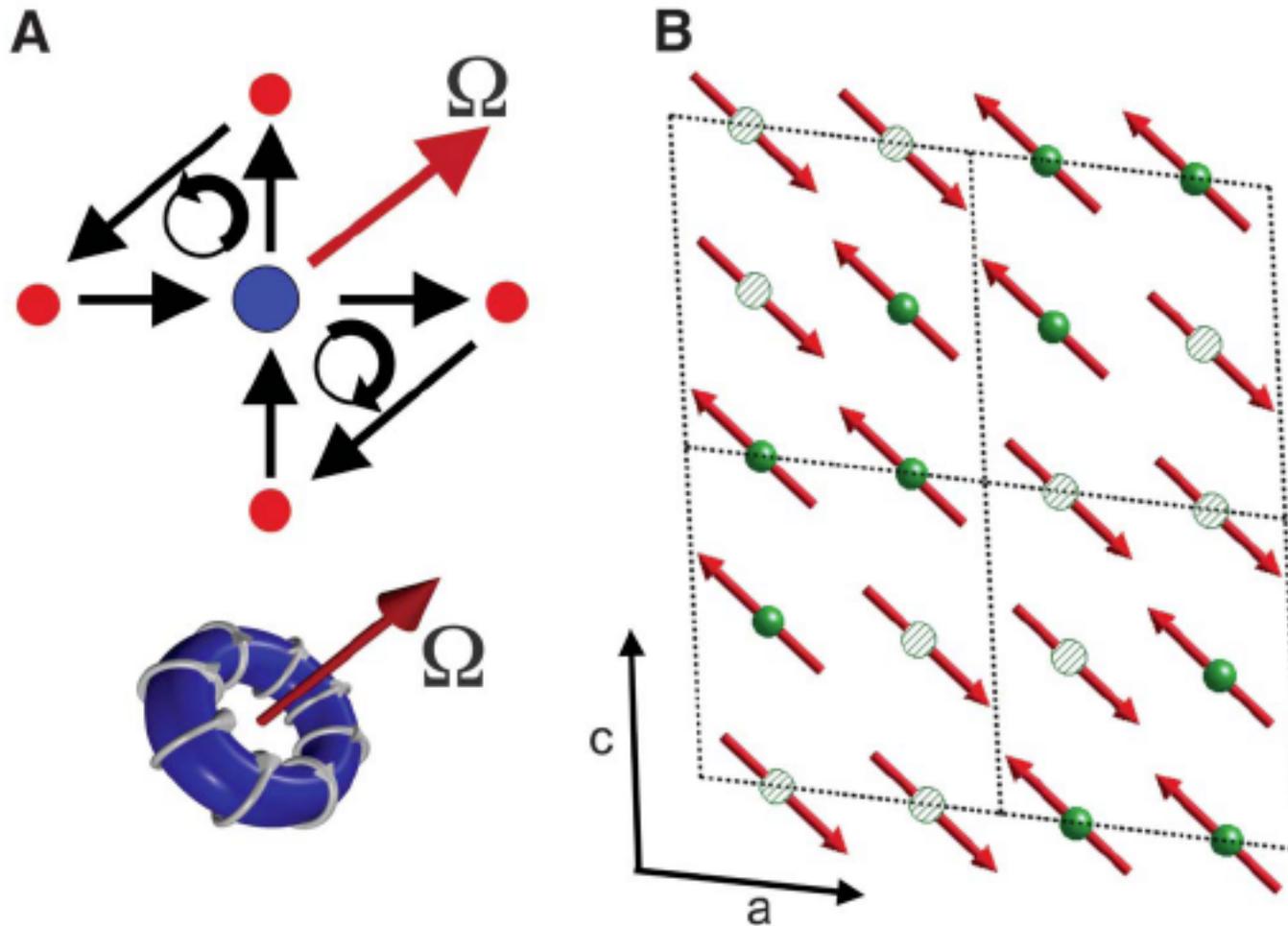
Scagnoli *et al.*, Science (2011)

Dichroism in CuO (commensurate AF phase)
 $\sin(2\psi)$ azimuthal dependence



Scagnoli *et al.*, Science (2011)

Toroidal Moments in the Commensurate AF Phase of CuO?



Dichroism due to E1-E1, E1-M1 interference?

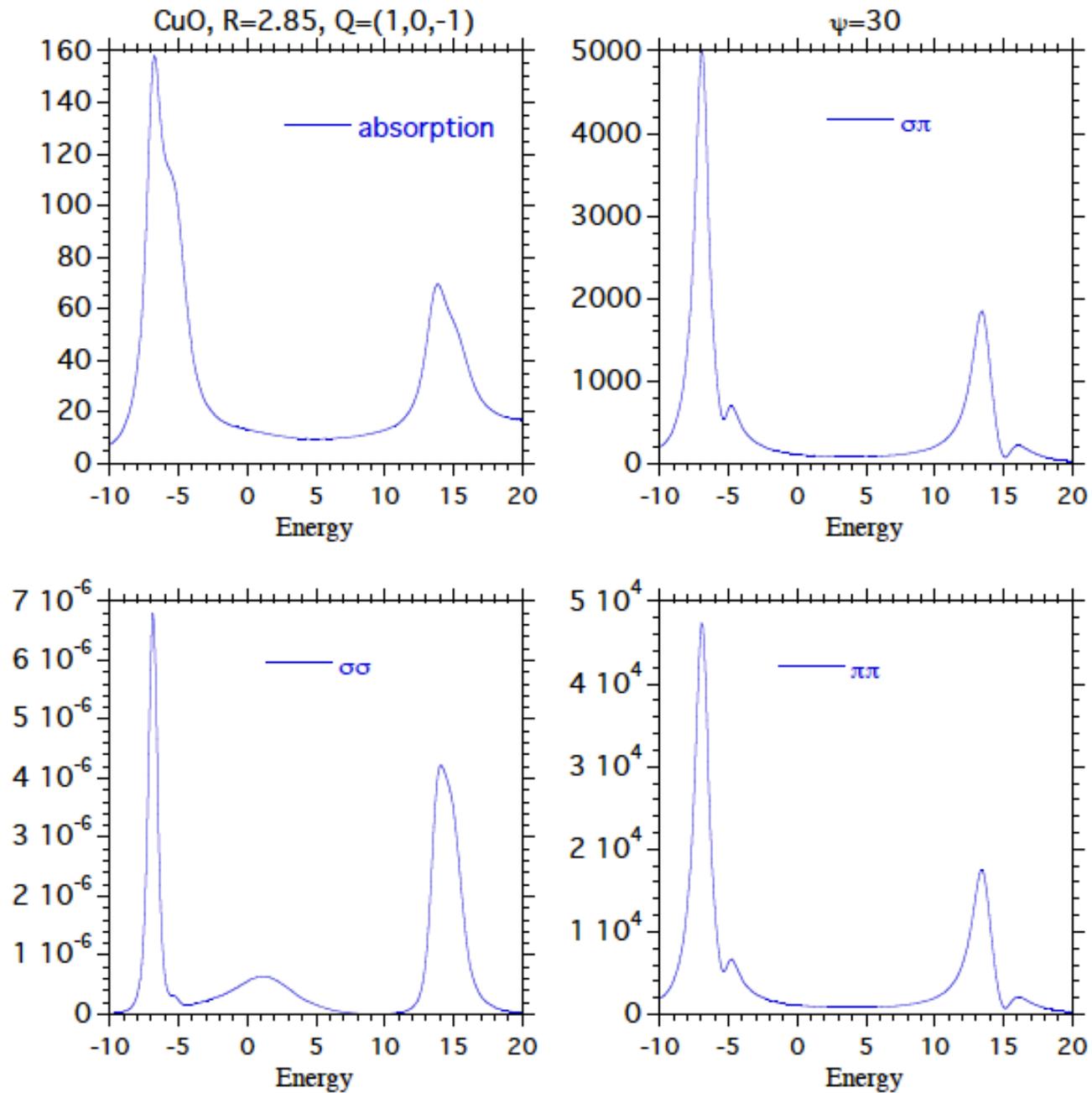
$$\begin{aligned}f_1^{\text{E1-E1}}(\sigma\sigma) &= 0 \\f_1^{\text{E1-E1}}(\sigma\pi) &= -im_y \cos\theta \cos\psi \\f_1^{\text{E1-E1}}(\pi\sigma) &= im_y \cos\theta \cos\psi \\f_1^{\text{E1-E1}}(\pi\pi) &= im_y \sin(2\theta) \sin\psi\end{aligned}$$

$$\begin{aligned}f_{1a}(\sigma\sigma) &= 2T_x \cos\theta \sin\psi \\f_{1a}(\sigma\pi) &= -T_x \sin(2\theta) \cos\psi \\f_{1a}(\pi\sigma) &= T_x \sin(2\theta) \cos\psi \\f_{1a}(\pi\pi) &= 2T_x \cos\theta \sin\psi\end{aligned}$$

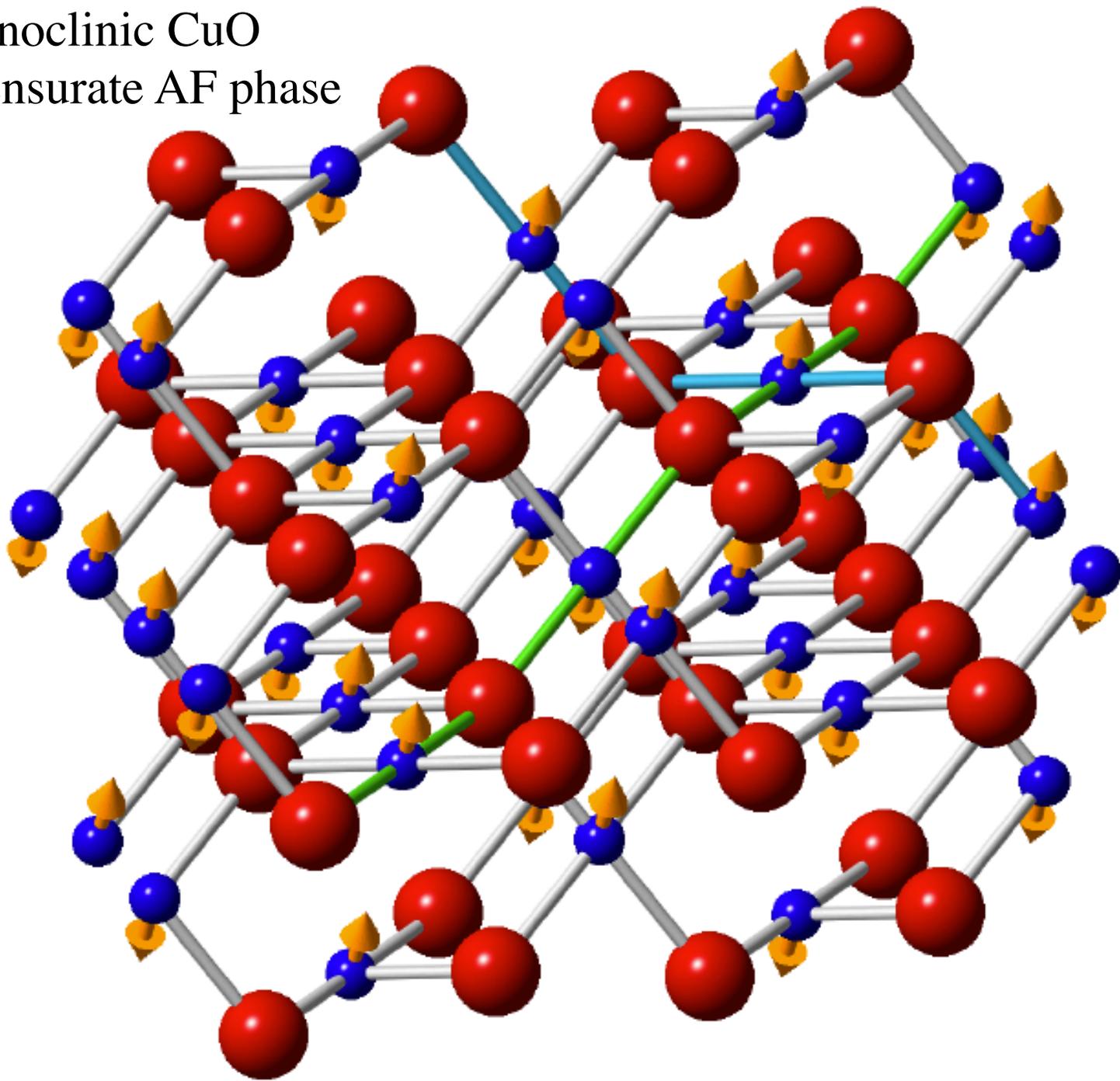
$$\begin{aligned}f_{1b}(\sigma\sigma) &= 2M_{yz} \cos\theta \sin\psi \\f_{1b}(\sigma\pi) &= M_{xy} \cos^2\theta \sin(2\psi) \\f_{1b}(\pi\sigma) &= M_{xy} \cos^2\theta \sin(2\psi) \\f_{1b}(\pi\pi) &= -2M_{yz} \cos\theta \sin\psi\end{aligned}$$

$$\begin{aligned}\Delta I &\propto m_y T_x \cos^4\theta \sin(2\psi) \\&+ m_y M_{xy} \cos^3\theta \sin\theta \sin(2\psi) \sin\psi\end{aligned}$$

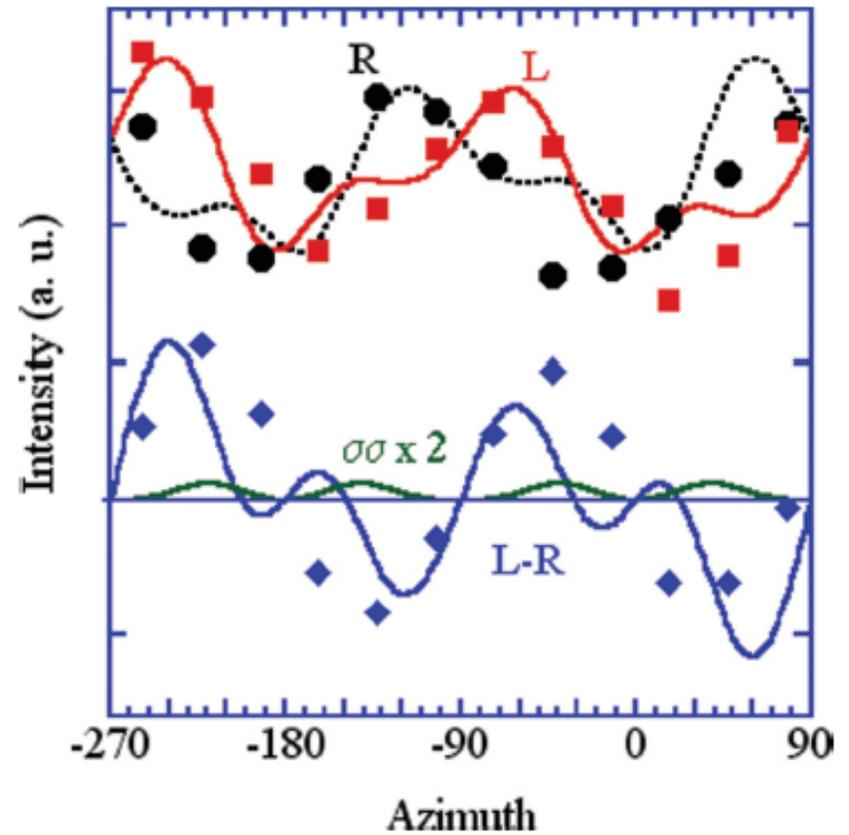
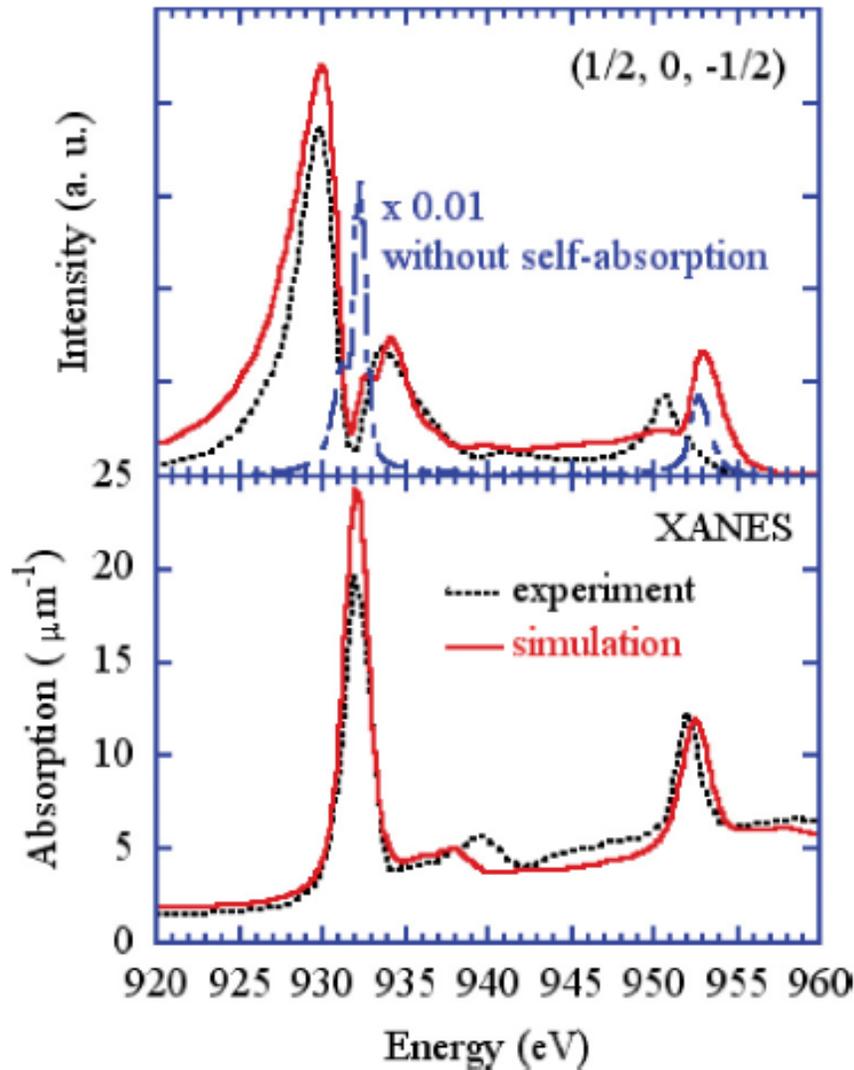
$\sigma\sigma$ scattering in RXD (due to E1-E2 terms) is $\ll \sigma\pi$ and $\pi\pi$ terms



Monoclinic CuO
Commensurate AF phase



Monoclinic structure leads to a rotation of the light (linear dichroism)
So $\sigma\sigma$ signal due to contamination from $\sigma\pi$ magnetic dipole contribution



Joly *et al*, PRB (2012)

$\sigma\pi$ scattering in RXD dominated by anisotropic charge scattering

Hg1201
Q=(100)
Cu K edge
AF oxygens
S along c axis

